

A NEW 1D BIOGEOCHEMICAL MODEL FRAMEWORK FOR ASSESSING AND MANAGING ACID SULFATE SOIL RISKS

by

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BACKGROUND

The biogeochemistry of acid sulfate soils is complex, involving oxygen transport into the sediment (required to oxidise pyrite), kinetically controlled reactions (e.g. pyrite oxidation, dissolved iron reactions), secondary acidification effects (e.g. acidic mineral formation, metal solubilisation), transport processes (e.g. leaching, diffusion to surface and ground water), and acid neutralisation reactions (e.g. sulfate reduction, carbonate dissolution). Currently, no single model is available that can adequately simulate all the potential processes influencing the biogeochemistry of acid sulfate soils. However, some models have been developed for oxidation and leaching processes of pyrite in mining contexts (Wunderly et al. 1996). The Simulation Model for Acid Sulfate Soils (SMASS) developed by Bronswijk and Groenenberg (1992) incorporates most relevant processes, but does not include many potentially important and more recently researched aspects (e.g. ion binding to dissolved and solid organic matter, clays and oxides). Recently, a multilayer model (SMARTml) has been developed to simulate acidification and the transport of nutrients and heavy metals in soil that includes these processes (Bonten et al. 2011). By coupling the SMASS acid sulfate soil model functionality to the SMARTml biogeochemical functionality, a powerful tool could be developed to simulate the biogeochemistry of acid sulfate soils and improve risk assessment and the management of their impacts.

The aims of this study were to: (a) describe the development of a new one-dimensional (1D) biogeochemical model framework for acid sulfate soils and (b) apply the model to simulate acid generation and drainage processes in an agricultural area in the Lower Murray River region of South Australia.

MODEL DEVELOPMENT

An outline of the model framework is presented in Figure 1.

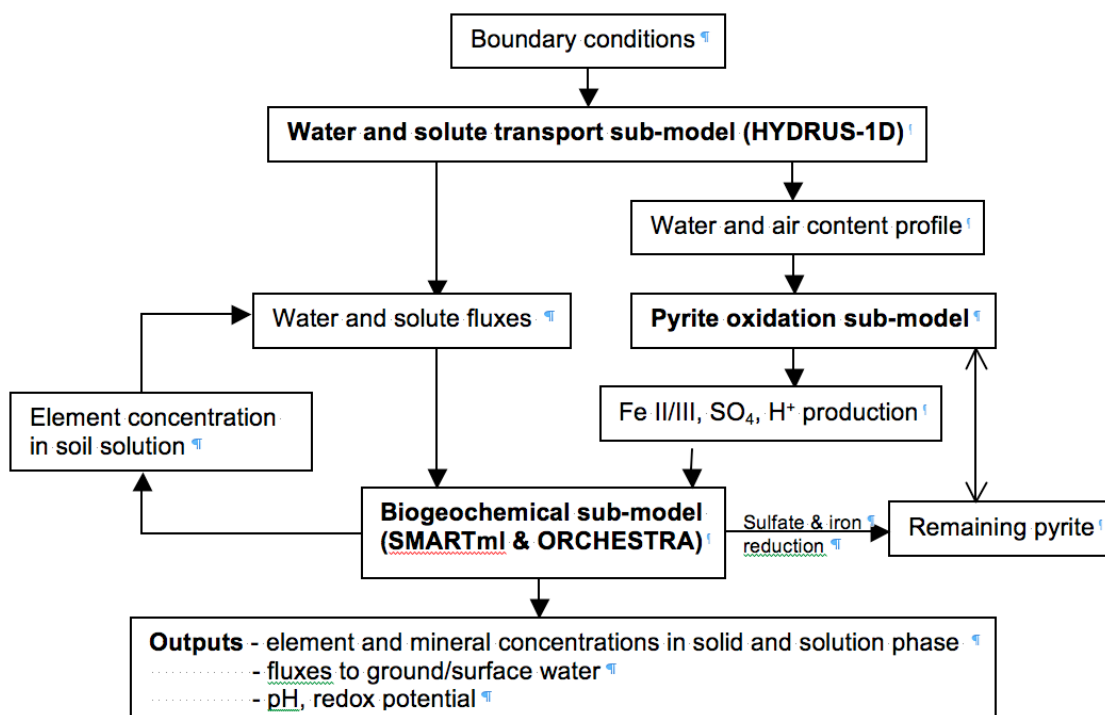


Fig. 1. Model framework

The following sub-models were coupled together (independently) to create a 1D model framework for simulating acid sulfate soil biogeochemical reactions and transport processes:

Water and transport sub-model - The widely used and supported model for water and solute flows in variably saturated media, HYDRUS 1D (Simunek et al. 2008), was used to provide moisture content and fluxes at various depths/ compartments in the soil profile. HYDRUS's graphical user interface enables schematisation of the soil profile, and the defining of different top and bottom boundary conditions (e.g. meteorological, irrigation, variable or constant pressure heads/fluxes, seepage faces, horizontal drains) and hydraulic properties.

Pyrite oxidation sub-model - The air content profile (= porosity - water content) in each soil compartment was calculated and the methods of Bronswijk and Groenenberg (1992) used to compute oxygen diffusion coefficients, oxygen consumption values (from pyrite oxidation and organic matter decomposition), rates of pyrite oxidation (also dependent on pyrite crystal size), and the concentration of pyrite oxidation products (Fe II/III, SO₄, H⁺) in each soil compartment. Oxidation and precipitation of monosulfides, FeS, can also be assessed if required.

Biogeochemical sub-model - The coupled SMARTml-ORCHESTRA models (see Bonten et al. 2011) were used to simulate the biogeochemistry of the soil profile subsequent to pyrite oxidation. First, the production/consumption terms for the non-equilibrium processes (such as iron and sulfate reduction) were calculated. The total concentrations of each chemical component were calculated in the soil compartments by summing the production/consumption terms, the inflow/outflow fluxes from the water and solute transport sub-model, and the total amounts from the previous time step. From these total concentrations, the equilibrium concentrations in the soil solution, the composition of the exchange complex, and the amount of mineral precipitates were computed for each compartment.

The coupled model utilises a daily time step, and multi-year simulations can readily be performed. The model is very flexible and capable of simulating a

wide range of acid sulfate soil issues and management scenarios (e.g. different irrigation or drainage regimes, addition of lime to soil).

MODEL APPLICATION EXAMPLE

Drought conditions and low inflows from 2006–2010 in the Murray-Darling system in Australia led to unprecedented low water levels in the lower reaches of the river. This resulted in groundwater tables falling under the adjacent agricultural areas (Lower Murray Reclaimed Irrigation Area, LMRIA). The heavy clay soils subsequently dried and cracked, resulting in pyrite oxidation in the sub-soil. The return of river and groundwater levels in late 2010 resulted in the appearance of acid drainage across an area of 3300 ha and resultant river water quality risks. There was a critical need to better quantify and model the biogeochemical processes in the LMRIA subsoils so that risk management could be improved. The new model described above was applied to simulate the pyrite oxidation processes, the mobilisation of acidic cations (H^+ , Al III, Mn II, Fe II/III), trace elements (e.g. As, Ni, Zn) and nutrients, and neutralisation (sulfate reduction) at a trial site.

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